

Sandia

R E S E A R C H

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ON THE COVER

Sandia's Hongyou Fan conducts a materials experiment in his lab. Fan, whose research focuses on assembly and engineering of nanostructured materials for device integration, has developed cutting-edge technologies and received awards including an R&D 100, Federal Laboratory Consortium Outstanding Technology Development and 2012 Asian American Engineer of the Year. Fan has been with Sandia since 2000. He is the author or co-author of 60 scientific papers and has more than 4,000 citations and 20 patents and patent applications.

(Photo by Randy Montoya)

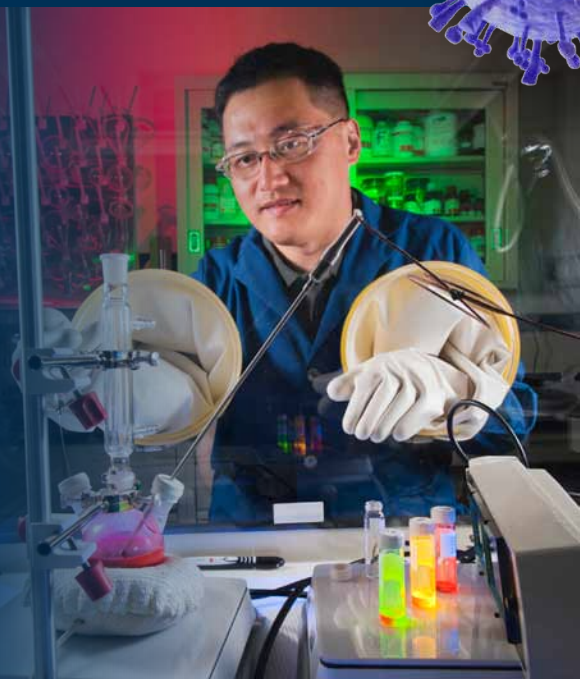
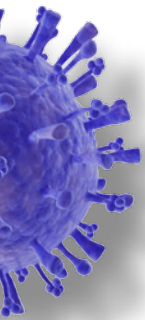
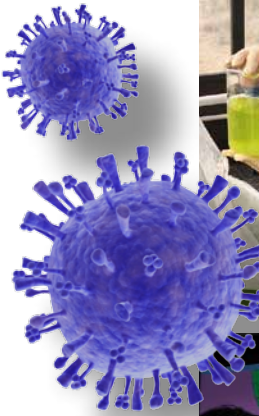
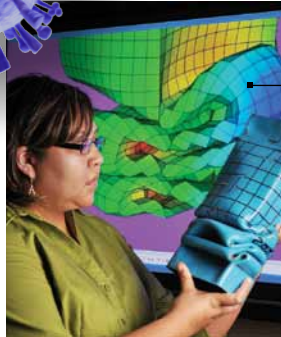


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SCIENCE IN SUPPORT OF NATIONAL SECURITY

During the course of Sandia National Laboratories' history, we have designed and developed more than 90 percent of the 6,500 nonnuclear components found in a modern nuclear weapon. We have also engineered a variety of other systems and technologies, from those that protect U.S. warfighters and the nation's infrastructure, to systems that detect a host of radiological and biological threats, to solutions that ensure clean, affordable, abundant energy.

The technical impact we have made and continue to make across the national security arena is underpinned by fundamental science and engineering research. Research that spans a spectrum of disciplines including

chemistry, physics, materials science, biology, geoscience, nanoscience, computer science...the list goes on. The ability to apply multiple research and development disciplines to solve complex national security problems is a defining feature of Sandia.

Research is intrinsic to our technological accomplishments. This research leads to greater understanding of physical systems, which in turn leads to novel applications in national security devices and systems. For example, when integrated circuit technology evolved from local oxidation to separate transistors to a high-density, shallow-trench isolation scheme, Sandia developed the scientific understanding required to modify the technology for demanding radiation environments. The technology now forms the basis of every radiation-hardened silicon CMOS (complementary metal oxide semiconductor) integrated circuit Sandia develops and produces for stockpile and space applications.

With this issue, we are excited to debut *Sandia Research* as a window into the scientific work that forms the basis of our national security mission. We spotlight the cutting-edge research performed in the Labs' seven research foundations: Bioscience, Computing and Information Sciences, Engineering Sciences, Geoscience, Materials Science, Nanodevices and Microsystems, and Radiation Effects and High Energy Density Science. In addition, readers will meet some of the talented scientists who find solutions to the critical issues facing our nation.

Readers will also learn why our research matters. Concerns like the effects of climate change, domestic and international terrorism, clean and affordable energy, and the safety, security and reliability of the nuclear deterrent are important to our nation's quality of life. The innovations and breakthroughs produced at Sandia tackle these and similar matters.

Sandia National Laboratories is a research and development laboratory that uses forefront science and engineering for the U.S. public good. We invite you to learn more in these pages.

— **J. Stephen Rottler**

*Chief Technology Officer and Vice President
Science, Technology and Engineering Research
Foundations*





SANDIA'S *headlights*



*Research
foundations
lead beyond
the known and
into tomorrow*

By Nancy Salem

Physicist Dick Claassen could not have imagined the magnitude of exploration he would set in motion when he penned a memo to colleagues at Sandia National Laboratories on May 31, 1957. World War II was history, the Cold War was reality and Sandia was in transition, its nuclear weapons mission shifting from production engineering and assembly to systems and product design.

Claassen envisioned a broader, more complex mission that called for deep roots in the fundamentals of science and engineering. His memo to Sandia leadership set out the characteristics and guidelines of a research organization at the Labs.

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INTRODUCTION

I would like to describe for you our plans, desires, and goals for a program in what we call fundamental physical sciences. I would like to do this in four parts, following a little background of material. First, I will try to describe the objectives; that is, those accomplishments which we hope to achieve by such a program; second, what I call the configuration of such a group; third, the method by which we have chosen the fields in which we will work; and fourth, two examples of specific programs which have already been initiated in this area.

Since the term "fundamental" and the term "science" are used in so many ways by different people, perhaps we should define first what we mean by "fundamental physical science". The real definition should be evident by the end of my talk, as determined by the boundary conditions we will place on this program and as exemplified by those programs which we can list. Briefly, however, let me say that by "fundamental physical science" we intend to imply research programs which will contribute new and original knowledge of phenomena in the fields of physics, physical chemistry, and to a lesser extent, electrical engineering and engineering mechanics.

As you are aware, Sandia Corporation has reached its present position as a research and development laboratory by a process of evolution. I believe it is pertinent to point out the relationship of this evolving pattern to our present plans for research activities. Originally, Sandia was a split from Los Alamos Laboratories, fostered mainly by geographic considerations. The primary reason for this was of matching into the military system, and it added the problem of production of engineering designs, partially completed elsewhere. Still, a variety of weapons designs has created

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"I would like to describe for you our plans, desires, and goals for a program in what we call fundamental physical sciences," the memo opened. Claassen wrote that Sandia's research efforts were a result of the development of nuclear weapons components. "In a mature organization, the research effort should be expended in advance of the development programs," he continued. "We are in an international weapons race. To obtain and maintain a superiority in this race, we must find a way to form a very close coupling between advances in fundamental knowledge and engineering designs of new weapons."

Claassen proposed research into electronics ("Semi-conductors are of high interest in many places in the country."), radiation effects, combustion, hydro-magnetics, theoretical mechanics, thermal shock and geophysics. He wrote that the choice of fields was crucial, "for if they are wrong, then even the best of research individuals cannot make effective contributions."

"These are a set of fields or disciplines or sciences which are the underlying basis for the solution of many practical development problems," he wrote.

Claassen got a thumbs-up from Sandia leadership and the job of establishing and leading the research

organization. He was promoted in 1960 to director of physical research, the first to hold that post.

Fast forward a half century to a Sandia Labs where fundamental research is at the heart of the Labs' national security mission and identity. The work takes place in seven research foundations, each focused on a specific scientific discipline and overseen by the Office of the Chief Technology Officer and the Research Leadership Team. "Research is the headlights of the Laboratory," says Steve Rottler, Sandia VP of Science & Technology and Chief Technology Officer. "We can look broadly across the scientific and engineering community and ask, 'What are the new and emerging areas of research that could have a beneficial impact on the nation?'"

A search for core competencies

The foundations had roots in Claassen's organization but didn't take shape as an entity until the early 1990s when then-Director Al Narath wanted to deepen the Labs' commitment to a vibrant research community in support of the mission. He asked a committee to identify Sandia's strengths based on the seminal Harvard Business Review article on core competencies by C.K. Prahalad and Gary Hamel.

The panel agreed on five core competencies: engineering science, materials science, pulsed power, microelectronics and photonics, and computing. The first research foundations were built around those disciplines. Over time the original foundations



evolved, names changed and new core competencies emerged, resulting in the current seven foundations: Bioscience, Computing and Information Sciences, Engineering Sciences, Geoscience, Materials Science, Nanodevices and Microsystems, and Radiation Effects and High Energy Density Science.

“The foundations exist to enable the mission and advance the frontiers of knowledge in science and engineering,” says Julia Phillips, Deputy Chief Technology Officer and director of Sandia’s Research Strategy and Partnerships center. “With high beams on we can see things that haven’t been articulated yet.”

Research supports national security in important ways, Phillips says. “It provides the opportunity to explore concepts that are farther out,” she says. “The time horizon is longer. There’s time to think about how to do something as opposed to being schedule-driven.”

Rottler says program work in a national laboratory is typically driven by near-term considerations. “You think in the lifespan of a program,” he says. “In the research community you have the luxury of being able to look out well beyond programs that are in place today, perhaps even envisioned. We can look into new and emerging areas that, if mastered by an adversary, could be used to the disadvantage of us



Sandia post-doctoral fellow Carlee Ashley, above, looks into the use of nanoparticles to blast cancerous cells with a mélange of killer drugs; researcher Xinjian Zhou, above right, was inspired by the human eye to build a nanoscale color detector; and principal investigator Curt Salisbury, below, challenges the dexterous robotic hand that he helped create.

and our allies. We can position ourselves to counter a threat if it becomes a reality.”

Rottler says both near- and long-term research are motivated by and vital to Sandia’s mission. “As an institution we become more appreciative of the life-cycle of research and the varying temporal scales,” he says. “Each of them is important to the future of the Laboratories.”

Research for the public good

Much of the funding for research in the foundations comes from Laboratory Directed Research & Development (LDRD), a \$165 million-a-year program that invests in staff-generated, high-risk, high-potential ideas that advance Sandia’s missions and scientific frontiers. Rottler calls LDRD a precious resource and the engine of research at Sandia.

“The reason it is so precious is we have considerable discretion over what we fund, with oversight from the National Nuclear Security Administration,” he says. “If we need a new capability to support our mission or



we want to start something new and expand our impact from a national service perspective, this funding makes that possible. Some of the biggest programs at the Labs today had their start in LDRD.”

LDRD and research in each foundation have helped Sandia attract and keep exceptional scientists. “One reason the Laboratory is what it is today is the people we hire. You can’t state it strongly enough,” Rottler says. “We attract professionals who are among the smartest people on the face of the planet, who are not afraid of challenging problems and who believe national service is worthy of a career commitment.”

Their work impacts the larger scientific, academic and business communities and, ultimately, people on the street through partnerships that produce invention, innovation, entrepreneurship and economic development. “We want to assure that the results of publicly funded research and development are deployed for the public good,” Phillips says.

Research results are published in peer-reviewed journals and contribute to the broad body of science and engineering knowledge, helping other researchers and stimulating creative thinking that builds on Sandia’s work. And a considerable body of research becomes intellectual property (IP) in the form of patents or copyrights available for licensing by industrial partners. IP with commercial potential moves from the Labs into the private sector and the hands of the


public. IP with national security implications is developed by industry for use by the government.

Ingredients of innovation

When Dick Claassen wrote about the importance of electronics and semiconductors back in the 1950s he might well have been peering into a crystal ball. His vision embodies why Sandia’s research foundations exist: to look ahead.

Claassen saw a future where tiny devices could change lives, and Sandia ran with it. Rottler says discoveries and innovations in microelectronics, microsystems and nanodevices are among the Labs’ greatest achievements. The Microsystems and Engineering Sciences Applications, or MESA, complex supports research and development programs throughout the Laboratories and is at the forefront of international advancement in the field. “I really believe that over the past 15 years this is something that has gone from being important to the Labs to being a cornerstone of the Labs,” Rottler says. “It’s incredible what comes out of that foundation every year in terms of advancement.

“This is an example of the outstanding things that can happen at a place like Sandia with sustained customer and leadership commitment over a long period of time. You assemble a critical mass of people and develop world-class facilities and you create a work environment in which truly innovative things can happen. They can’t happen any other way.” ■



New realms beckon the phenomena of *life*

By Stephanie Hobby

National security was once largely the domain of physicists and chemists, but events such as the anthrax attacks in 2001 and the H1N1 influenza pandemic in 2009 have driven biologists to the forefront of national security. Sandia's newest research foundation, Bioscience, is taking on a key role as the nation looks increasingly to biology for solutions to its national security challenges.

The challenges revolve around biodefense and bio-energy. Solutions come from about 100 Sandia scientists and engineers from New Mexico and California who apply a combination of 'omics' (genomics, proteomics, etc.), biomolecular imaging, computational biology and microfluidic approaches to increasing knowledge about how microbes and microbial communities work.

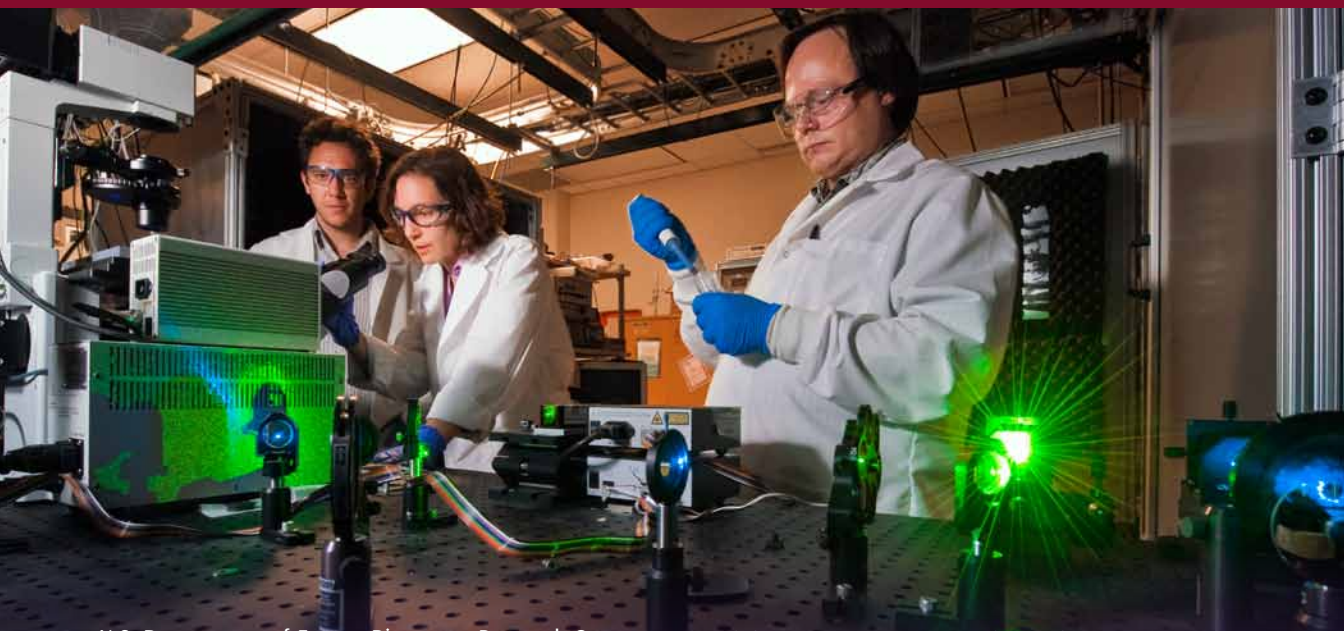
"Sandia is a national security laboratory, and our nation faces significant national security challenges

that biology must address," says Malin Young, lead director of the Bioscience Research Foundation.

"Infectious disease and the threat it poses, whether spread accidentally or deliberately, is a serious concern. In addition, our nation is highly dependent on external energy sources, and biofuels are an important way to enhance our energy independence."

Foundation research into biofuels and biodefense makes important contributions to the nation's body of knowledge. Sandia researchers work to reduce U.S. dependence on foreign oil by focusing on transportation biofuels derived from cellulosic and algal biomass. Developing such clean, renewable and efficient sources of domestic energy will reduce the nation's need for foreign oil and boost economic and military strength.

Sandia is a key partner at the Joint BioEnergy Institute, a



U.S. Department of Energy Bioenergy Research Center in Emeryville, Calif. JBEL's mission is to perform the research to produce advanced biofuels. Sandia and the National Renewable Energy Laboratory are partners in the Sustainable Algal Biofuels Consortium led by Arizona State University to monitor the health of algal ponds and catch potential problems early, and Sandia is a partner in the Sapphire Energy Inc.

Integrated Biorefinery Project, both funded by DOE. And Sandia scientists are making significant progress in studying nutrient recycling to encourage efficient growth and development of biomass.

"The bioscience program is performing work that ranges from monitoring the health of algal ponds, to finding methods to deconstruct biomass, to engineering organisms to produce biofuels," Young says. "We also focus on understanding disease mechanisms and developing medical diagnostics and detection systems that will augment our ability to respond to outbreaks."

Defending against biological weapons and understanding how new diseases emerge and propagate are still relatively new focuses in national security. Sandia scientists have broken barriers in imaging techniques to produce never-before-seen images of how immune cells interact with and respond to diseases such as plague. Sandia's Rapid Threat Organism Recognition system, or RapTOR, is changing the way scientists and health professionals identify known diseases and characterize new pathogens. Able to sensitively detect trace amounts of pathogens in clinical samples, RapTOR is funded by DOE, the Department of Defense, and the Department of State, and further commercialization opportunities abound. RapTOR originated in Sandia's Laboratory Directed Research & Development (LDRD) program.

From left, Jesse Aaron, Jeri Timlin and Bryan Carson work with new super-resolution imaging techniques to view cell-level activity with unprecedented detail. Their research supports Sandia's biological threat reduction programs.

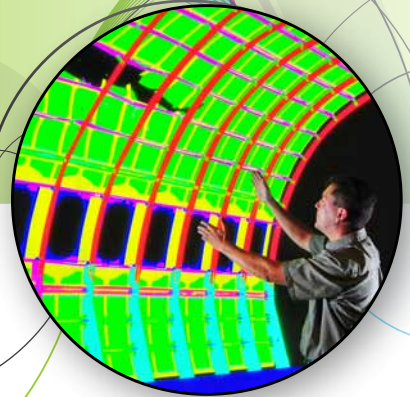
"There's tremendous potential for biology to impact national security missions in biodefense and biofuels areas," Young says. "Our focus now is to develop an integrated approach to getting information about biological systems at different molecular and cellular levels. Integrating that multi-dimensional data will provide our researchers with new and actionable insights about how biological systems function. We aim to apply that knowledge to develop new countermeasures for pathogens and to develop new approaches to biofuel production and scale-up." ■



Field engineer Brian Dwyer takes an algae sample as part of a project to create alternative sources of energy. Sandia teams are cultivating green algae as a promising new supply of biofuel.

BITS and BYTES LINK THE GAMUT OF RESEARCH

By Neal Singer



The wide range of the Computing and Information Sciences (CIS) Research Foundation includes cybersecurity, engineering research and advanced computational capabilities.

“Our work integrates efforts across much of the Labs,” says foundation lead Director Rob Leland.

CIS’s long-range focus is to help advance science and engineering processes within an overarching framework that extends computing capabilities beyond the completion of particular objectives. The goal is to surmount the usual technical limitation of tackling only tasks specific to a mission goal.

Because each of Sandia’s seven research foundations makes ample use of computing, says Leland, “CIS offers a Labs-wide capability that provides a gentle force for overall cooperation and alignment.”

At one level, CIS links computing sciences — the design of computing machines and processes — with informa-

tion sciences that involve the analysis, classification, manipulation, retrieval and dissemination of information.

To ensure privacy for these and other Sandia endeavors, CIS has tripled the number of Sandia organizations involved in coordinating cybersecurity and is reaching out to cyber researchers in academia and industry for new ideas and qualified people to bring to the Labs. These moves, says Leland, “represent an expansion of mission emphasis in this key realm.”

CIS’s work has national security implications because information is increasingly substituted for both materials and energy to increase the efficiency of various processes. Computerized telemetry, for example, is used to distantly observe a site rather than travel to it, or create meetings to which participants do not travel but instead are linked electronically by telecommuting. The method also allows researchers to observe interactions among simulated molecules under difficult conditions without building a “wet” lab or running explosives tests.

Because computation has become a fundamental tool of science, it does more than complement theory and experiment in areas where experimentation is difficult, expensive, impossible or prohibited.

Improvements for engineering science at Sandia include a computer-aided design tool for quantum computing (QCAD), analogous to the more familiar CAD tools used in



building and tool design. The new tool is used to simulate electrical devices whose behavior strongly depends on quantum effects, especially quantum dots that rely upon the action of one or a few electrons. “The capability enables rapid modeling to accelerate the design of a silicon quantum dot qubit,” manager John Aidun says of reactions involving only a few electrons.

At the high end of supercomputing CIS’s goal is, first, to support efforts to supplant the transistor after its successful 50-year run and then to create an exascale computer design that will achieve a billion operations a second without sucking up the energy needed by a small city.

“Our goal is a new device ‘family’ with vastly superior properties that should replace the conditions of Moore’s law,” Leland says. The startlingly accurate law has been valid in predicting computing-speed

increases directly related to the shrinking of the size of the circuits. “But in 10 to 15 years, the features of a device will be only a few atoms across. It’s hard to conceive how you could go beyond that with current technology.”

Leland envisions a continuation of the technical journey that substituted transistors for vacuum tubes. New devices will be sandwiched between stacked chips, transmitting information using photons instead of electrons. “That will reduce heat losses

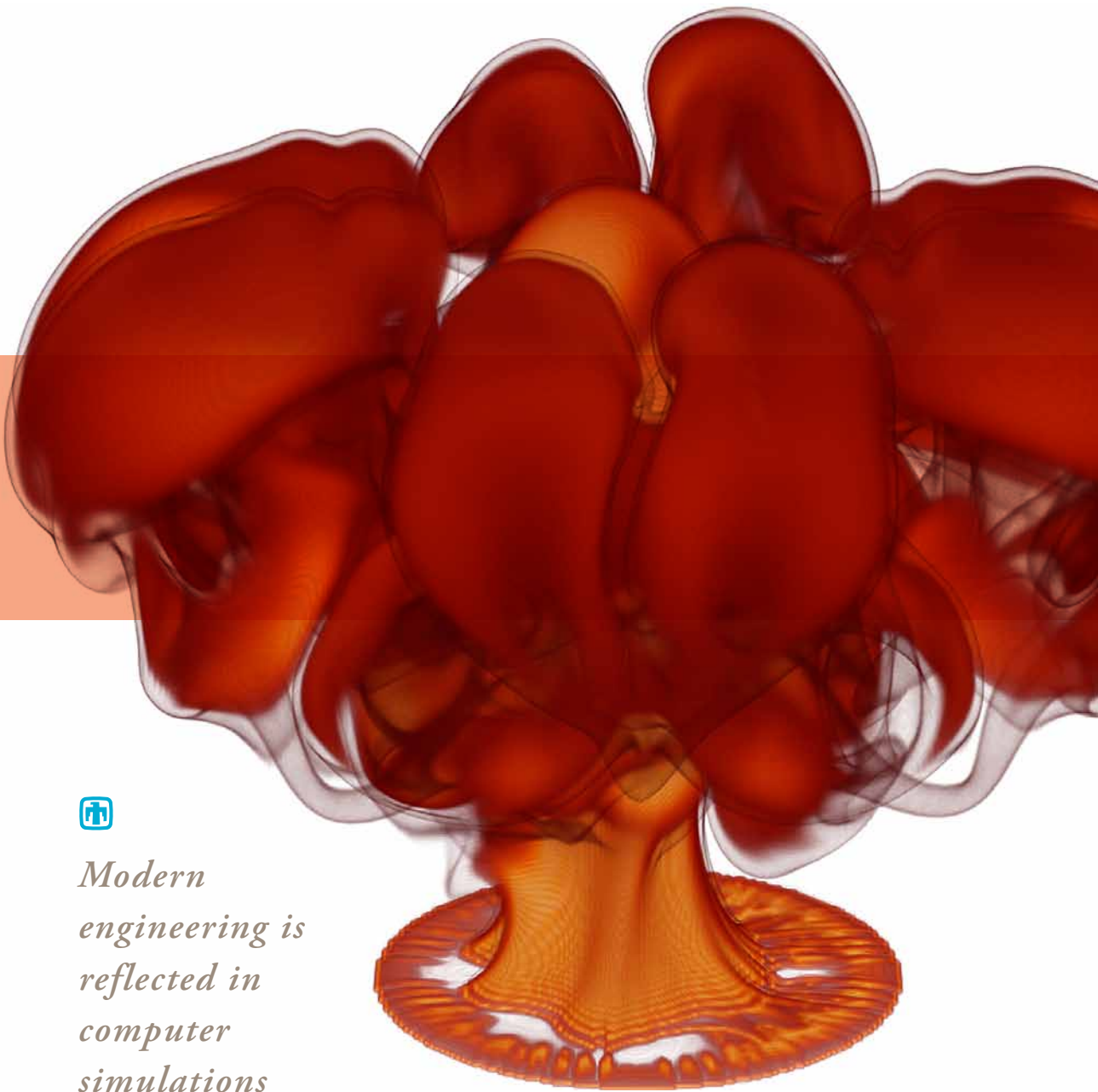


Sandia researchers, from left, Archie Gibson, Jeff Gruda, Don Rudish, Ron Minnich and George Bachand use cutting-edge computing tools to advance science and engineering across the Labs and beyond particular objectives. Their work ranges from supercomputing to cybersecurity and quantum computer-aided design.

and energy costs,” Leland says. “The economics are not yet compelling but they will be.”

The lengthy, guided technical journey toward the exascale supercomputer is “one reason why we have a research foundation,” Leland says.

Sandia’s computing work has been impressive, bringing on line Paragon, the first parallel processing computer; ASCI Red, the first teraflop computer; and a revolutionary design for a supercomputer called Red Storm that became the most reproduced supercomputer on the planet. ■



*Modern
engineering is
reflected in
computer
simulations*

It's hard to imagine a major program at Sandia that doesn't work with the Engineering Sciences Research Foundation for its skills in computational engineering analysis and sophisticated experimental testing and evaluation.

"We offer expertise from several technical organizations in solid mechanics, structural dynamics, combustion, thermal science, fluid mechanics, aerodynamics, energetics research, electromagnetics/electrical sciences and shock physics. We focus not only on fulfilling current program requirements but also anticipating what is needed in the future," says Duane Dimos, director of the Engineering Sciences Center in Albuquerque and lead director of the research foundation.

Modern engineering is driven by computational simulations, which in turn depend on experiments to provide vital data and validate the range within which the models can be used reliably.

"Our codes support calculations for complex problems, such as evaluating the response of a nuclear weapon during launch and reentry environments, which can only be done on the latest high-performance computers," Dimos says. "In partnership with the Computing and Information Sciences Foundation, we've defined a leadership position in computational analysis, because we have difficult problems to address and we've developed these engineering codes to solve them."

Combining computational and experimental simulation enables researchers to improve designs, analyze performance margins and assess the safety and reliability of components and full systems. “Our unique experimental capabilities, which can simulate extreme environments such as the effect of a lightning strike or being engulfed in a jet fuel fire, support the modeling and give us confidence about the way we’re doing things,” Dimos says.

Engineering Sciences touches programs across Sandia, from defense systems such as satellite payloads, hypersonic vehicles and rail guns to energy systems such as engine efficiency and wind turbine performance and homeland security concerns such as aircraft safety or improvised explosives.

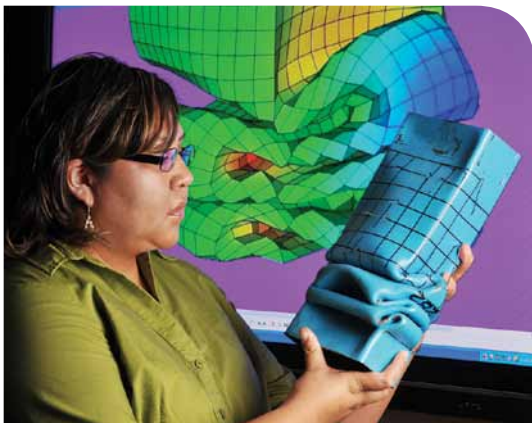
At the Labs’ Combustion Research Facility, a DOE Office of Science Collaborative Facility, researchers are developing validated simulation codes for next-generation

COMPLEX PROBLEMS NEED *Sophisticated Solutions*

By Sue Major Holmes

The foundation’s research capabilities have their roots in work on the nation’s nuclear weapons program. The level of computational and experimental expertise was a natural outgrowth of the need for greater amounts and precision of data after underground nuclear testing ended in 1992. DOE investments in high-performance computers helped increase Sandia’s computational expertise.

Today, researchers in engineering sciences are deeply involved in programs to modernize the nuclear stockpile. “We will be relied on to provide critical support for the design, development and qualification of these modernized weapon systems,” says Russ Miller, director of the California Weapon Systems Center, which is part of the research foundation. “The analysis, tests and understanding engineering sciences provide will be critical to our success in this endeavor.”



Modeling and simulation are increasingly important fields as engineers like Sandia’s Jhana Gorman tackle problems involving multiple scales of time and size.

engine designs. “We are developing new experimental diagnostics to inform and validate code development,” says Bob Carling, director of the Transportation Energy Center, part of the foundation at Sandia’s Livermore site. “Our work on high-pressure engine performance will lead to innovations and more efficient vehicles.”

Engineering Sciences partners with the Materials Science Research Foundation to understand how manufacturing variations can impact the performance of critical components for Sandia’s work, Dimos says. An important example is efforts to develop performance models for explosives and pyrotechnics, which will improve the ability to design components that use such energetic materials.

“We need to account for the complex interaction between chemical reactions and energy release in energetic materials to determine component performance margins,” says Anthony Medina, director of the Energetic Components Center, which is in the research foundation. “Our goal is having experimentally validated models that also account for long-term effects due to material aging.”

Other organizations recognize Sandia’s computational expertise and have adopted Sandia computer codes for their use, most notably its Sierra Mechanics code. “An outstanding example comes from the 18-year partnership with Goodyear, which is adopting a version of Sierra Mechanics for tire design. Having our codes in use by others challenges us to continue improving,” Dimos says. “We are also making Sandia codes increasingly available through open-source distribution to benefit the entire engineering community.” ■

Where Earth INTERSECTS Engineering

By Nancy Salem

Sometimes what's below the surface can illuminate what's above. The Geoscience Research Foundation at Sandia Labs digs into Planet Earth for knowledge that sheds light on concerns from climate and energy security to disaster response and clandestine underground facilities.

"Our work is about solving national security problems that involve the Earth and atmosphere," says foundation lead Director Marianne Walck. "We focus on sub-surface properties, structure and processes, surface and atmospheric phenomena, and how engineered systems interact with the Earth system."

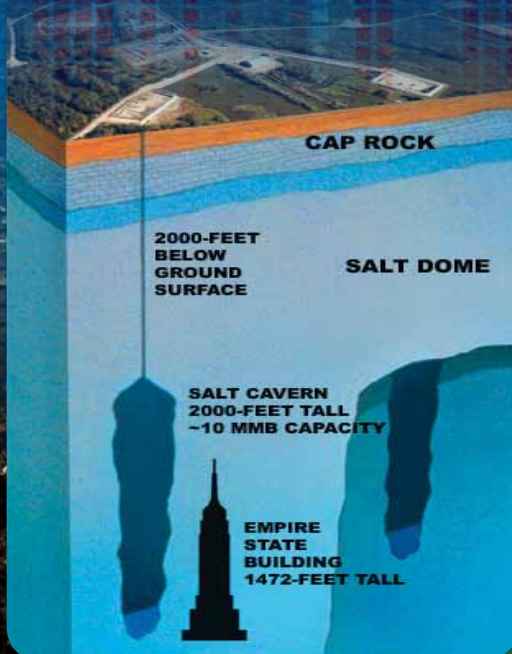
The scope of research extends to water use and quality; carbon capture, reuse and sequestration; energy production, storage and security; defense and intelligence; nuclear weapons; nonproliferation; disaster response; and climate security.

"What makes us different from most of Sandia is we address problems that intersect with Earth systems," Walck says. "We deal with things that have to do with physics, chemistry and biology, but all relating to the Earth and atmosphere instead of engineered materials or systems."

Geoscience research was established at Sandia in the late 1950s, primarily to study the effects of atmospheric and underground nuclear weapons testing. That quickly evolved into methods to determine the size of the weapons' seismic yield and into global monitoring of nuclear tests for treaty verification.

"We did almost all the close-in measurements of underground nuclear tests right up until testing stopped in 1992," Walck says.

In the 1970s what is now the U.S. Department of Energy asked national laboratories to use technologies



developed for weapons programs to address the energy crisis. Sandia geoscientists studied oil shale and underground radioactive waste disposal, becoming a major player in the DOE's Waste Isolation Pilot Plant near Carlsbad, N.M., and later the Yucca Mountain Project proposed for Nevada.

"We started with weapons and that translated into energy," Walck says.

Geoscience Foundation research continues to support nuclear test ban treaty verification through seismic and infrasound measurement, as well as other national security missions including the detection of underground facilities that manufacture and/or store weapons of mass destruction.

Sandia is the scientific adviser to DOE on the Strategic Petroleum Reserve in such areas as cavern design and

integrity, oil temperature and geologic study. The reserve of about 700 million barrels is stored in deep engineered caverns dissolved out of salt domes along the Texas and Louisiana Gulf Coasts.

The Labs' Atmospheric Radiation Measurement Facility near Barrow, Alaska, monitors the atmosphere daily, collecting data to improve climate models. And Earth systems research advances natural disaster response by measuring how utilities, roads and other infrastructure react to such events as earthquakes and hurricanes.

A project at Barrow measures atmospheric radiation, particularly in arctic clouds. "These are different from clouds in Albuquerque. They contain ice, which changes their properties," Walck says. "Climate effects are amplified at the poles. We're trying to understand the whole system of how ice clouds might behave and affect how the Earth warms and cools at high latitudes."



Sandia's Anna Snider Lord and Chris Rautman combine geologic and other data, such as well logs and oil industry seismic surveys, to map the deep engineered domes of the Strategic Petroleum Reserve.

In the realm of basic energy sciences, foundation researchers are studying how shales and mudstones release oil and gas when fractured. "We're trying to understand the properties of shales and mudstones at levels not yet studied," Walck says. "We previously

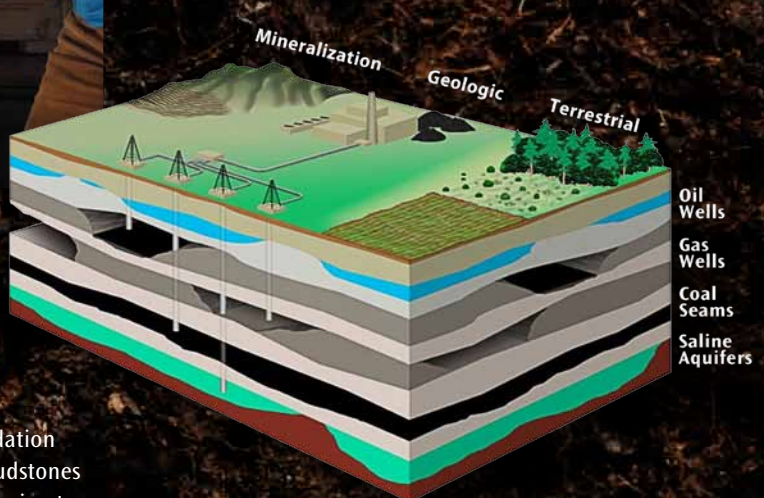
didn't pay much attention to these kinds of rocks. We're now using advanced techniques to understand and learn more."

Researchers look at how fluids move through the rocks, and use focused ion beams to create microscopic pillars of shale to see how they respond to mechanical stresses. "We're doing some very cool stuff through imaging," Walck says. "This work is about opening new energy resources."

Another project is molecular modeling of rock/fluid interactions. "This builds understanding at the molecular level of how fluids in geomaterials interact with minerals," Walck says.

The work is relevant to carbon-dioxide sequestration, in which CO₂ could be removed from the atmosphere and stored in underground reservoirs. "One question is what happens when you put the carbon dioxide in the rock system? How does it interact with what's down there?" Walck says. "We look at it at the molecular scale and use that information to predict what will happen at the larger scales, all the way up to the size of a reservoir, several kilometers across."

Understanding natural systems such as the Earth is fascinating and challenging. They are heterogeneous, and their behavior is difficult to predict, Walck says. "Sandia excels at investigating these types of tough, interdisciplinary issues. The combination of our earth science expertise with Sandia's engineering base provides the know-how for tackling big problems at the complex intersection between the Earth system and the engineered environment." ■



Subsurface layers could play a role in carbon-dioxide sequestration, the transfer of CO₂ from the atmosphere into underground reservoirs.



**How does
a carbon,
glass or metal**

BEHAVE?

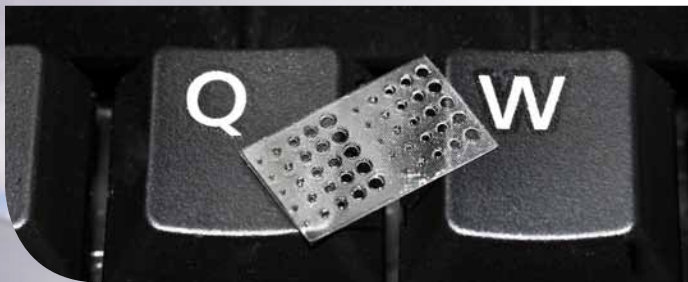
By Sue Major Holmes

Materials science doesn't often lead a project, but it is always a critical part of Sandia's national security mission.

Scientists and engineers couldn't do their work without materials ranging from ceramics to polymers to semiconductors to thermoelectrics, says Carol Adkins, lead director of the Materials Science Research Foundation, which melds broad capabilities in materials.

A goal of materials science research is being able to predict how various materials will behave. Accurate predictions rely on the ability to model, simulate, understand and describe the fundamentals of materials, backed by experiments to verify the models, Adkins says.

"What material should I use? How will it interact within this system? Will it perform as I need it to in the



Materials scientists fabricated this tiny test structure, shown here on keyboard keys for scale, as part of a neural interface project aimed at improving amputees' control over prosthetics with direct help from their own nervous systems. The structure helped researchers test a way to manufacture the interface.

expected environments – not only now, but decades in the future? Those are key questions,” Adkins says. “We not only have to improve our understanding of today’s materials, but keep our eyes on the horizon for new material needs.”

Work encompasses everything from the materials science necessary to qualify microelectronics in radiation environments for the nuclear weapons program to synthesizing specialty organic materials for sensors or predicting performance uncertainty for stainless steel welds, she says.

Five thrusts, under the umbrella of prediction, describe the research: performance and reliability; control of energy, mass, and charge transfer; next-generation materials for electronics and optoelectronics; computational materials synthesis and processing; and developing novel characterization tools and techniques.

Materials science work grew out of Sandia’s nuclear weapons mission, and Adkins says that’s still a critically important customer. The foundation supports all of Sandia’s missions and is a strong player in its Laboratory Directed Research and Development program, which invests in higher-risk projects to advance science. Materials Science also partners with the Engineering Sciences Research Foundation to understand materials from the atomic to the continuum scale, and with the Nanodevices and Microsystems Research Foundation to understand the role of materials in device performance.

However, no single area of work funds more than half of Sandia’s materials research “so we work hard to maintain a vibrant body of fundamental materials science work for diverse customers,” Adkins says.

The face of materials science at Sandia is changing as one generation retires and another takes its place. Experts with 20-plus years of experience built on strong science are leaving. “With today’s tools, we can be even more predictive than we’ve been in the past, relying

less on directly applicable experience,” Adkins says. “Our new staff members are eager to take our fundamental understanding to the next level. It’s the wave of the future.”

Because materials science is so pervasive, it’s also strongly collaborative. The foundation includes the Materials Science and Engineering Center directed by Adkins; the Physical, Chemical and Nano Sciences Center directed by Charles Barbour, both at Sandia/New Mexico; and materials experts at Sandia/California led by Malin Young of the Biological and Materials Science Center. Anthony Medina from the Energetic Components Center and Thomas Zipperian from the Responsive Neutron Generator Product Deployment Center are also involved.

The foundation wants to foster an atmosphere where people “are free to think new and exciting thoughts about science and to explore and discuss new things” and where the science, engineering and product delivery sides of a problem understand each other and work together, says Barbour.

“Collaboration at the Labs makes things happen, but if the only goal is collaboration, I don’t think that’s enough,” he says. “We need a vibrant research environment to address missions. We’re always striving for that.”

The Internet has fostered new ways of collaborating. For instance, Sandia researchers in California can remotely operate the state-of-the-art aberration-corrected scanning transmission electron microscope housed in New Mexico. Sandia has other “fabulous tools” for materials research, including the Ion Beam Laboratory, microelectronics silicon and compound semiconductor fabrication labs and the Sandia/Los Alamos Center for Integrated Nanotechnology (CINT), a Department of Energy Office of Science center, Adkins says.

“Sandia’s New Mexico and California sites work as one lab in materials science with our jointly operated characterization tools and the breadth of our work and responsibilities,” she says. ■



Teeny-tiny scales yield

huge payoffs

By Sue Major Holmes



*New behaviors,
radical change*

Two individually powered nanowires are embedded one above the other in the atomic layers of a Sandia-grown crystal. This unique test device has produced new information about nanoworld electrical flows.

Sandia's Nanodevices and Microsystems Research Foundation works at the smallest of scales to spur imaginations on the grand scale, and does that partly through what Gil Herrera, the foundation's lead director, calls "an amalgamation of competencies."

"We foster the intermingling of people representing a number of disciplines from across the entire laboratory who understand a variety of different scientific and engineering disciplines at great depth," he says. "It really is allowing people to imagine and come up with wonderful innovations."

The foundation is responsible for fundamental microsystems research and development, engineering design, component engineering and semiconductor manufacturing. It works with other national laboratories, federal agencies and industry.

But the idea isn't simply to take things in the macro-world and shrink them. Rather, it's to understand the physics that occurs at very small scales that doesn't occur at the macroscale.

"We're trying to create new behaviors of devices and systems and create new performance that's the direct result of these very small scales," says senior manager Wahid Hermina.

Light and matter, for example, can be coupled much more strongly at tiny scales, or researchers can manipulate how acoustic waves travel through materials when they work from the fundamental properties of those materials, he says.

And there are what engineers call quantum effects that occur at nano scales. That opens the door to really radical change: Instead of trying to find a behavior or a material in nature with the necessary properties, researchers can design the needed behavior by tailoring the material or leveraging phenomena at the nanoscale.

"All of a sudden you've created something that doesn't occur naturally, engineered from the basic building blocks of understanding at these micro- and nanoscales, and that could be plentiful and available," Hermina says. "The sky's the limit. That's what we're in the business of doing here. We're trying to create devices and systems that provide new opportunities for a vast segment of the national industrial base."

Sandia pioneered work in microsystems in the 1960s with the invention of the laminar flow clean room. It went on to establish leadership in radiation-hardened integrated circuits, institute revolutionary work in superlattices that deliver the framework for custom semicon-

ductor materials, develop groundbreaking capability in novel microsensors and microsensor systems, and create and improve a variety of chemical and biological detection systems.

Microelectronics capabilities stem from Sandia's nuclear weapons mission, which remains a primary responsibility. The research foundation focuses on broader national security challenges, Herrera says.

The people behind the research need state-of-the-art facilities for their mission, so the foundation is based in Sandia's 400,000-square-foot Microsystems and Engineering Sciences Applications complex of laboratories, clean rooms and offices. MESA brings together scientific disciplines to produce integrated microsystems, and is the only microelectronic foundry producing chips hardened to survive a nuclear battlefield or other intense radiation environments.

Researchers under the foundation also use the Center for Integrated Nanotechnology, a Department of Energy science center operated jointly by Sandia and Los Alamos national laboratories; the Ion Beam Laboratory, Sandia's unique applied physics lab with six particle accelerators; and individual laboratories throughout Sandia.

Herrera can point to recent projects arising from the foundation or in which it played a major role: microsystems-enabled photovoltaics, dubbed "solar glitter," that combine mature technology with advances in photovoltaic cell design; breakthroughs in solid state lighting; and a microsystem neuroprobe that can be inserted into the brain without causing cellular damage.

"MESA has been responsible for some really cool innovations," he says.

The foundation has been involved in 41 R&D100 awards won by Sandia. It also has participated in, although not necessarily led, most of Sandia's Grand Challenge Laboratory Directed Research & Development projects, Herrera says.

It tackles large tasks because of its multidisciplinary strength and its flexible facilities that enable people to develop their ideas, all without interfering with the mission to provide trusted and secure weapons components, he says.

"It's all based on the principle that with the best facilities, you can attract the best people and the best partners throughout Sandia, in universities, companies and other labs. It's amazing what happens when you combine incredible innovators and world-class facilities," Herrera says. ■



The first letter of this alphabet is

Sandia's mission to certify the nation's nuclear stockpile as safe, secure and effective requires understanding the science that underpins the design, performance and aging of nuclear weapons components and systems in the absence of underground testing.

That mission comes into focus in the Labs' Radiation Effects and High Energy Density Science (REHEDS) Research Foundation, where researchers are developing the scientific understanding needed to certify that nuclear weapons will operate as intended. The foundation has a multitude of projects in radiation-material interactions, dynamic material properties, radiation physics, pulsed power fusion and pulsed power science and technology.

It works in three main areas: radiation effects science and engineering, high energy density science and pulsed power science and technology.

The foundation is advancing radiation effects science and engineering to ensure systems work despite being bombarded by everything from X-rays to gamma rays to neutrons.

High energy density science, defined as the study of materials at pressures greater than 1 million atmospheres, applies to nuclear and non-nuclear components of a weapon and "involves creating extreme states of matter at very high temperatures and pressures to validate physics models that are used to certify the stockpile," says Keith Matzen, the foundation's lead director.

The pulsed power science and technology element of the research foundation develops methods and facilities to create these extreme conditions for nuclear weapons research in the laboratory.

Sandia is home to the Z facility, which includes the Z pulsed-power generator — the largest lab-based pulsed-power facility in the world — coupled with the Z-Beamlet and the Z-Petawatt lasers. Matzen says that while the lasers are not unique by themselves, their combination

with the Z pulsed-power generator creates unique experimental capabilities for dynamic material properties, effects of low energy X-ray photons on weapon components and pulsed-power fusion studies.

"The focus is using the unique energy efficiency and pulse length of the Z facility to perform experiments that are complementary to experiments using lasers," he says. "We've obtained some very exciting and important results in all of these research areas."

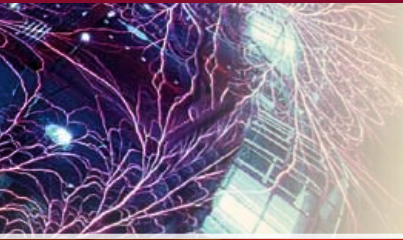
Pulsed-power facilities in the Radiation Sciences Center include HERMES III, the world's most powerful gamma simulator, and Saturn, which studies effects of high energy X-ray photons on electronics and materials in weapon components. The center also operates the Annular Core Research Reactor and the Gamma Irradiation Facility, which produce intense neutron and gamma-ray environments.

REHEDS relies on other Sandia capabilities as well, including the Physical, Chemical and Nano Sciences Center's Ion Beam Laboratory. "While it's not in and of itself a radiation effects or high energy density science environment, ion beam sources can be used to simulate neutron-material interactions that are important to radiation effects science," Matzen says.

The stockpile is not the only research area with an interest in extreme environments. Other defense and commercial systems must operate despite intense radiation, Matzen says. "In addition, we must make sure adversaries don't gain a technological advantage in these focus areas, and we must apply our scientific understanding to the areas of nuclear nonproliferation and counterproliferation," he says.

The foundation also collaborates extensively on projects with universities and other national laboratories.

"We encourage interactions with universities in fundamental science, particularly astrophysics and planetary science," Matzen says. "For example, researchers at several



Physicist Ryan McBride pays close attention to the tiny central beryllium liner to be imploded by the powerful magnetic field of Sandia's Z machine. The larger cylinders forming a circle on the exterior of the base plate measure Z's load current by picking up the generated magnetic field.



By Sue Major Holmes

universities have been excited by experiments showing that our facilities can provide the laboratory-based access to the environments found in the photospheres of white dwarf stars, which have been used as chronometers for the age of the universe. Similarly, we have interactions with academic researchers investigating the opacity of elements in the sun, with the goal of understanding the solar structure in terms of its temperature and density profiles.”

While university collaborations in fundamental science represent only a small fraction of the Z facility’s experimental effort, “they help attract young scientists into the important research areas of the research foundation as well as bringing new ideas for using our laboratory capabilities to better understand extreme environments,” he says. ■

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LOOKING BACK

The idea seemed so simple to Willis Whitfield that he didn't think it was an invention. He couldn't believe someone hadn't thought of it. To keep a room very clean, let air be the janitor — a “janitor” sweeping the premises every six seconds.

The modern electronic age as we know it began in the early 1960s when Willis, a Sandia Labs physicist, envisioned using fans not only to send outside air through filters into a room but also to remove the air in equal measure through exhaust pipes in the far wall.

The omnipresence of the technique today in hospital surgery units, electronics plants and laboratories makes it easy to take the “clean room” invention for granted. Things were different back then.

“I was amazed at the high level of interest,” Willis said. So-called clean rooms of that era had no control over their own air, and depended solely on masks, gowns and janitorial services.

“They were looking at the wrong things,” Willis said. When he checked for dust contamination in the prototype clean room, “the particle counter just stopped counting. We thought there was something wrong with it,” he said. The Sandia prototype room was 1,000 times cleaner than any ever measured.

A statue of Willis, who passed away Nov. 12, 2012, at age 92, stands outside Sandia's MESA facility as a monument to the visionary, pioneering work of one man and the legacy of scientific research at Sandia Labs.

— Neal Singer

